

# Acetic acid

# 5-acetoxy-4-methoxy-tetrahydro-pyran-3-yl

InChI: InChI=1S/C10H16O6/c1-6(11)15-8-4-14-5-9(10(8)13-3)16-7(2)12/h8-10H,4-5H2,1-3H3  
InChIKey: PHXHFIHKPNANIV-UHFFFAOYSA-N

Formula: C10H16O6

SMILES: COC1C(OC(C)=O)COCC1OC(C)=O

Mol. weight [g/mol]: 232.23

## Physical Properties

Property code	Value	Unit	Source
gf	-616.61	kJ/mol	Joback Method
hf	-989.91	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	62.90	kJ/mol	Joback Method
log10ws	-0.14		Crippen Method
logp	-0.105		Crippen Method
mcvol	167.520	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpola	1479.89		NIST Webbook
rinpola	1479.89		NIST Webbook
tb	640.36	K	Joback Method
tc	847.49	K	Joback Method
tf	394.48	K	Joback Method
vc	0.614	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.79	J/molxK	640.36	Joback Method
cpg	482.87	J/molxK	674.88	Joback Method
cpg	498.07	J/molxK	709.40	Joback Method
cpg	512.36	J/molxK	743.92	Joback Method
cpg	525.70	J/molxK	778.44	Joback Method
cpg	538.07	J/molxK	812.97	Joback Method
cpg	549.43	J/molxK	847.49	Joback Method
dvisc	0.0013874	Paxs	394.48	Joback Method

dvisc	0.0008679	Paxs	435.46	Joback Method
dvisc	0.0005885	Paxs	476.44	Joback Method
dvisc	0.0004244	Paxs	517.42	Joback Method
dvisc	0.0003211	Paxs	558.40	Joback Method
dvisc	0.0002524	Paxs	599.38	Joback Method
dvisc	0.0002046	Paxs	640.36	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R268143&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R268143&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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